LA-UR-22-20477

Approved for public release; distribution is unlimited.

Title:	2022 Agnew and Metropolis Postdoc Fellow Showcase Event Book
Author(s):	With, Mary Anne Whalen
Intended for:	Showcase event in person and on Webex on 1/27/22
Issued:	2022-01-20

2022 Agnew and Metropolis Postdoc Fellow Showcase Event Book

Agnew & Metropolis Postdoc Fellow Showcase

Thursday, January 27, 2022
12:30 p.m.

Jemez & Cochiti Meeting Rooms
and
Webex

POSTDOC PROGRAM

Harold Agnew National Security Postdoctoral Fellow

Agnew National Security Postdoc Fellows pursue cutting-edge experimental, theoretical, computational science, and engineering research aligned with the national security mission:

- **Matter in Extreme Environments:** *Understanding the dynamic evolution of matter and its properties at high density, high temperature, and other extremes.* Key research areas include dynamic materials science (with an emphases on polymers, high explosives, metals, and actinides), fluid dynamics, high energy density physics (with emphases on radiation transport and plasmas), nuclear physics, inertial confinement fusion, and advanced manufacturing. The study of stellar astrophysics from star formation through stellar end states provides a natural laboratory for extreme environments some of which are also accessible through laboratory experimental facilities.

  This area also includes advances of accelerator methods, technologies that enable new diagnostics (including x-ray and proton radiography and neutron diagnostics), and data analysis of matter in extreme environments for current and future facilities such as DARHT, LANSCE, U1a, NIF, Z, APS, and LCLS.

- **Data Analytics:** *Techniques and tools to analyze and understand data sets so large and/or complex that traditional data processing applications are inadequate.* Advances in this area include methods to extract knowledge from multiple and diverse data sources, including physical sensor output, streaming data, social media, and other data sources. Tools that could be applied include signal processing, image processing, uncertainty quantification, machine learning, anomaly recognition, and data fusion. Data Analytics can be applied to both Matter in Extreme Environments. It also extends to security of cyber-physical networked systems, including threat detection and mitigation, especially prevention of surreptitious process modification and information transfer.

- **Advanced Engineering Analysis** — Exploration of finite element analysis, with an emphasis on the development of techniques that incorporate plasticity, creep, and damage of materials and participation in experimental activities to characterize relevant mechanisms and validate constitutive models. Practice of multi-disciplinary engineering methods, including High Explosive Engineering, Complex Systems Engineering, Nuclear Safety and Surety Engineering, Modeling and Simulation of Complex Systems, and their application to issues in Stockpile Stewardship. This area also includes extreme engineering for deployment of autonomous measurement systems to remote, harsh environments such as space.

Agnew National Security Postdoc Fellow Presenters

Eric Bryant, W-13 / EES-17

co-mentored by Nathan Miller, W-13 and Kane Bennett, EES-17

Alex Cleveland, Q-5

co-mentored by David Chavez, Virginia Manner and Chris Snyder, Q-5
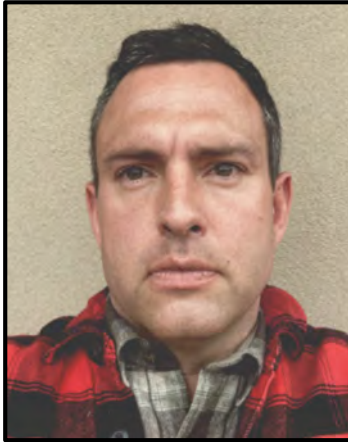
Samantha Couper, M-9

mentored by Blake Sturtevant, M-9

Ida DiMucci, C-IIAC / C-AAC / C-PCS

*co-mentored by Stosh Kozimor, C-IIAC, Angela Olson, C-AAC
and Ben Stein, C-PCS*

Belinda Pacheco, M-9 / Q-5

*co-mentored by Shawn McGrane, Cindy Bolme and John Lang, M-9
and Kyle Ramos, Q-5*

Eric Bryant, W-13 / EES-17

Eric is a postdoc in the Advanced Engineering Analysis (W-13) Group within the Weapon Systems Engineering (W) Division and the Geophysics (EES-17) Group within the Earth and Environmental Sciences (EES) Division. He investigates computational modeling of granular materials with a focus on coupled nonlinearities, as he previously did as a Presidential/Guggenheim and a Fertl Graduate Fellow at Columbia University (adv. WaiChing Sun) and the University of Texas (sup. Mukul Sharma), respectively. Eric joined the Laboratory in October 2020, initially in affiliation with the Center for Nonlinear Studies, and is presently researching higher-order continuum formulations for polymer-bonded particulate materials, derived by homogenizing inter-granular contact mechanics.

Eric received a B.S. in Civil Engineering from the University of Massachusetts Amherst, a M.S. in Petroleum and Geosystems Engineering from the University of Texas at Austin, and a Ph.D. in Civil Engineering and Engineering Mechanics from Columbia University in the City of New York. Eric is co-mentored by Nathan A. Miller in W-13 and Kane C. Bennett in EES-17.

Construction of a Micromechanics-Based Material Model for PBX

A general framework to derive nonlinear elastic and elastoplastic macroscopic material models from granular micromechanics is proposed. Like classical grain contact-based homogenization methods, reference solutions for closed-form hyperelastic material models are analytically derived from the grain-scale contact mechanics. However, unlike prior methods, the proposed homogenization framework defines an incremental variational principle that renders the traditional solutions extensible to plastic solids, i.e., closed-form hyperelastoplastic material models. The proposed framework is used to develop a novel granular micromechanics-based macroscopic model for pressure-sensitive Drucker-Prager plasticity with cross-linked grain-contact cohesive-debonding, as well as a combined model for damage, viscoelasticity, and viscoplasticity in polymer-bonded particulate materials like polymer-bonded explosive (PBX). Macroscopic inelastic continuum parameters are explicitly related to their microscale counterparts, e.g., the friction coefficient governing grain-scale inter-particle slip. Numerical examples and comparison to measurements from the literature, including compression and tension tests of pure concretes and PBX, in addition to finite element method (FEM) simulations of PBX boundary value problems, are used to investigate model predictions and demonstrate calibration to experimental data.

Alex Cleveland, Q-5

Alex is a postdoc in the High Explosives Science and Technology (Q-5) Group within the Weapon Stockpile Modernization (Q) Division. His research focuses on the development of novel, high-performing energetic materials that serve as potential replacements for conventional high explosives. Alex is a native of East Tennessee and has gradually moved west during his scientific training, ultimately joining the Laboratory in June 2020.

Alex received his B.S. in Chemistry from Tennessee Technological University and his Ph.D. specializing in Organic Chemistry from Louisiana State University. He is co-mentored by David Chavez and Chris Snyder of Q-5.

Synthesis and Unexpected Reactivity of a 1,2,4-Triazine Derived Azidoxime

The development of new energetic materials revolves around the design and synthesis of a compound that is predicted to have better performance, higher thermal stabilities, and lower sensitivities than current state-of-the-art explosives. Frequently the design and development of new materials is met with unexpected challenges such as failed reactions, complex mixtures of products, and the formation of unknown compounds.

In this presentation we will present the unexpected reactivity challenges of a 1,2,4-triazine derived azidoxime. This material was formed in three steps from a known triazine in a 64% combined yield and was subjected to acid catalyzed cyclization conditions in an attempt to form its 1-hydroxytetrazole isomer. However, this azidoxime failed to react even after prolonged reaction times or under heating. This unexpected result led us to probe the reactivity of this material computationally, through a surface analysis, and electrostatic potential mapping. This presentation will present our findings.
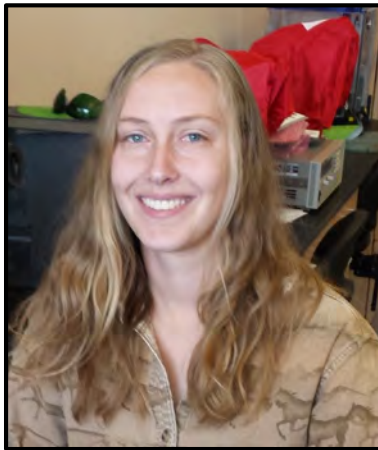
Samantha Couper, M-9

Samantha is a postdoc in the Static High Pressure Team of the Shock and Detonation Physics (M-9) Group within the Dynamic Experiments (M) Division. The focus of her M.S. geologic studies was on the magmatic evolution of the Bruneau Jarbige caldera, a ~13- to ~8-million-year-old precursor to modern day Yellowstone in 2016. Interest into the origins of deep magmatism led Samantha to pursue a PhD in high pressure geophysics,. For her doctoral research, Samantha applied novel methods such as double-sided laser heating in radial diffraction geometry, resistively heated radial diamond anvil cells (DACs), and polycrystal plasticity modeling of low-symmetry, multiphase materials. She joined the Laboratory in May 2021. Samantha's research focuses on experimental developments to high temperature resistive heating experiments and measurements of elastic constants on small samples (<40 µm) at high pressure in the DAC, thereby expanding both the accessibility and capability of simultaneous high P/T research in the DAC. Successful technique developments will be employed to study a variety of Group IV transition metals at high pressure for the first time.

Samantha received a Bachelor of Science in Geology from the University of California, Davis, and M.S. and PhD in Geophysics from the University of Utah. She is mentored by Blake Sturtevant of M-9.

Material Properties at Ultrahigh Pressures: Developing a Gigahertz Ultrasound Transducer for the Diamond Anvil Cell

The behavior of materials is governed by their environments: a material's structure and other properties readily change under varying pressure, temperature, and strain rate conditions. In a laboratory setting, phase transitions at higher pressures are often probed in-situ with an X-ray source. However, measurement of material properties is inhibited by the inverse relationship between pressure and sample size. Conventional ultrasonic techniques used on samples held at ambient conditions have wavelengths too long for the 25-100 µm samples necessary to achieve high pressures. To achieve shorter wavelengths (i.e. gigahertz frequencies), we are developing a piezolectric ZnO transducer that can be interfaced with specialized electronics to meet the demands of miniscule DAC samples. By altering the electrode design contacting the transducers, both shear and compressional waves can be created from the same transducer. The combination makes comprehensive measurements of material properties possible in-situ at high pressure and temperature and expands the probable pressure, temperature, and strain rate regimes necessary for modeling and interpreting both geologic processes and LANL mission critical materials at extreme pressures and temperatures.

Ida DiMucci, C-IIAC / C-AAC / C-PCS

Ida DiMucci is a postdoc in the Inorganic, Isotope, and Actinide Chemistry (C-IIAC) Group within the Chemistry Division where her work focuses both on photochemical transformations as well as X-ray studies of molten salts. DiMucci's Ph.D work, under the mentorship of Kyle Lancaster at Cornell University, focused on XAS studies of first row transition metals and earned her an ACS-DIC Young Investigator Award in spring of 2021. She joined the Laboratory in August 2020.

Ida received her BS in Chemistry from Gettysburg College and her PhD at Cornell University. She is co-mentored by Stosh Kozimor of C-IIAC, Angela Olson of C-AAC and Ben Stein of C-PCS.

Photochemical Separation of Plutonium and Uranium

Advancing actinide separations by reducing processing hazards is important for virtually all plutonium-based technologies. In many separations the strong reducing or oxidizing agents used are not always compatible with processing facilities and waste streams. Herein, we demonstrate that photochemical methods can be used in place of chemical redox agents in plutonium and uranium separations. Using UV-Vis analyses we determined that photoreduction from Pu^{4+} to Pu^{3+} and UO_2^{2+} to U^{4+} proceeded under ambient conditions in $HCl_{(aq)}$ and $HNO_{3(aq)}$. The photogenerated $Pu^{3+}_{(aq)}$ could then be separated from $U^{4+}_{(aq)}$ using anion exchange chromatography with high recoveries (>90% yield) and high separation factors (>9). This highlights usage of photochemical methods to improve safety, time efficiency, and effectiveness of plutonium and uranium separations.

Belinda Pacheco Johnson, M-9 / Q-5

Belinda is a postdoc in the Shock and Detonation Physics (M-9) Group within the Dynamic Experiments (M) Division and the High Explosives Science and Technology (Q-5) Group . She is originally from Muleshoe, TX. In her graduate work, Belinda developed a tabletop technique for in-situ imaging and temperature measurements of individual high explosive crystals initiated by shock waves. She joined the Laboratory in October 2021. Her research couples dynamic compression experiments to time-resolved spectroscopic probes for studying the chemistry and kinetics of high explosives.

Belinda received her B.S. in Chemistry at Texas Tech University, and a Ph.D. in Materials Chemistry at the University of Illinois at Urbana-Champaign. She is co-mentored by Shawn McGrane, Cindy Bolme and John Lang of M-9, along with Kyle Ramos of Q-5.

Benchtop Temperature Measurements in Shocked High Explosives

Experimental, time-resolved temperature measurements in shocked high explosives (HE) are elusive, and yet vital for validating reactive burn models used to understand HE performance. Optical and spectroscopy-based diagnostics are ideal for generating these data because of their high time resolution and ability to directly observe the extreme environments generated during shock compression. In this work we plan to couple high-throughput, laser driven flyer plates with Raman thermometry to simultaneously shock single crystals of 1,3,5,7-Tetranitro-1,3,5,7-tetrazocane (HMX) and collect *in-situ* shock temperatures. This benchtop-scale technique will enable the temperature measurements on a statistically significant number of samples at multiple impact conditions. Ultimately, these data will provide fundamental observables to the computational community which are needed for creating next-generation, predictive reactive burn models.

Current and Past
Agnew National Security Postdoc Fellows

Name	Postdoc Org(s)	Current Org
Barber, Jeffrey	DX-2	N/A
Barber, John	T-14 T-1/INST-OFF	T-1
Ben-Benjamin, Jonathan	P-4 EES-17 CCS-3	P-4 EES-17
Bielenberg, James	ESA-MEE	N/A
Billow, Brennan	C-IIAC B-11	MST-7
Bone, Sharon	C-IIAC RSO	N/A
Branch, Brittany	M-9 M-DO A-2	N/A
Brown, Katie	WX-9	N/A
Bryant, Eric*	W-13 EES-17	W-13 EES-17
Cleveland, Alexander*	Q-5	Q-5
Couper, Samantha*	M-9	M-9
Densmore, Crystal	C-ACT	N/A
DiMucci, Ida*	C-IIAC C-AAC C-PCS	C-IIAC C-AAC C-PCS
Duke, Dana	P-23	P-1
Fox, David	B-8	C-AAC
Fredenburg, David Anthony	WX-9	OES
Freeman, Matthew	P-25 P-23	P-1
Fry, Cathleen	P-27	P-3
Furlanetto, Michael	P-23	ALDPS
Jackson, Scott	DE-9	M-9
Kelly, Keegan	P-27	P-3
Kuvin, Sean	P-27	P-3

*Current Agnew Fellow

Current and Past
Agnew National Security Postdoc Fellows
Continued

Name	Postdoc Org(s)	Current Org
Leftwich, Megan	P-23	N/A
Mack, Nathan	C-CDE	A-2
	WX-6	
Manner, Virginia	WX-9	Q-5
McNeil (Vogan), Wendy	P-23	M-3
Meyer, Edmund	T-1	A-2
Murphy, Michael	W-6	Q-6
	Q-5	
Nguyen, Thuy-Ai (Bi)	C-IIAC	Q-5
Nizolek, Thomas	MST-8	SIGMA-2
Orlicz, Greg	P-23	NEN-3
	M-9	M-9
Pacheco Johnson, Belinda*	Q-5	Q-5
Pigott, Jeffrey	M-9	N/A
Quenneville, Jason	X-1-SMMP	N/A
	C-IIAC	
Schrell, Samantha	MPA-11	N/A
Tappan, Bryce	DX-2	Q-5
Veauthier, Jacqueline	C-IIAC	C-IIAC
	LANSCE-DO	
Volz, Heather	NMT-16	Q-18
	N-2	
Wallace, Mark	ISR-1	GS-IET
Welch, Cynthia	LANSCE-12	MST-7
Williamson, Todd	C-ADI	A-2
Wohlbier, John	ISR-6	N/A
Yeager, John	WX-9	Q-5
Zellner, Michael	P-23	N/A
	ISR-3	
Ziemann, Amanda	ISR-2	ISR-3

*Current Agnew Fellow

Nicholas C. Metropolis Postdoctoral Fellow

Metropolis Postdoc Fellows pursue cutting-edge research in the areas of computational and computer science, physics, and engineering. Computer simulation capabilities are developed in support of the stockpile stewardship program together with broader national nuclear security needs. Fellows have access to some of the most powerful supercomputers in the world to perform pioneering research in these disciplines.

- Research into complex, multi-physics, integrated numerical simulations and algorithms, including efficient use of advanced architectures for multi-physics codes.

- Development, validation, and incorporation of new physics and engineering models for integrated codes. These models include research into fluid mechanics, turbulence, microscopic and macroscopic models of material properties, warm dense matter, high explosives, plasma, nuclear, and atomic physics, and the transport of particles and x-rays.

- Development and application of fundamental physics codes to investigate relevant physics phenomena in these disciplines, including efficient use of advanced architectures.

- Verification and validation methodology and application, including development of a technically rigorous foundation to assess the confidence of simulation code results.

- Computer science and system development, including emerging technologies and investigation of advanced architectural concepts, system software, programming models, advanced storage and networking technologies, system and application resiliency, and numerical algorithms; system and application co-design for emerging technologies.

Metropolis Postdoc Fellow Presenters

Kevin Larkin, XCP-1 / XCP-5

co-mentored by Miles Buechler, XCP-1 and Abigail Hunter, XCP-5

Ben Southworth, T-5 / CCS-2

co-mentored by David Moulton, T-5 and James Warsa, CCS-2

Kevin Larkin, XCP-1 / XCP-5

Kevin Larkin is a postdoc in the Lagrangian Codes (XCP-1) and Materials and Physical Date (XCP-5) Groups within the X Computational Physics (XCP) Division. As a graduate student, Kevin joined the nonlinear dynamics and energy harvesting laboratory at New Mexico State University (NMSU), where he conducted research into modeling nano-sensors and energy harvesters. In 2018, Kevin began his work at LANL as a student guest with XCP-1 where he worked on implementing brittle fracture models in LANL's research code, FLAG. He is currently working on implementing a framework for viscoplastic models and strength models in FLAG.

Kevin received his B.S and PhD in Mechanical Engineering from New Mexico State University and is co-mentored by Miles Buechler of XCP-1 and Abigail Hunter of XCP-5.

Implementation of a New Rate-dependent Dislocation Density Evolution Model for Simulating Metallic Microparticle Impacts

Accurately modeling the rate-dependent plastic deformation of metals across a large range of strain rates requires a comprehensive accounting of dislocation motion and evolution. The newly developed analytical dislocation evolution model of Hunter and Preston, accounts for a wide range of dislocation annihilation and nucleation mechanisms including: network storage, Frank-Read sources, cross-slip, double cross-slip, mobile-immobile annihilation, grain boundary storage, grain boundary nucleation, and shock induced nucleation. In conjunction with the mean first passage time flow stress model, this new model is able to capture the plastic behavior of polycrystalline FCC metals across a large range of loading regimes from quasi-static to shock loading environments. These models have been recently implemented in Los Alamos National Laboratory's hydrodynamics research code, FLAG. Data from quasi-static, Hopkinson bar, and flyer plate experiments are used to create material parameter sets. Then continuum scale microparticle impacts are simulated in FLAG and compared to experimental observations.

Ben Southworth, T-5 / CCS-2

Ben Southworth is a postdoc in the Applied Mathematics and Plasma Physics (T-5) Group within the Theoretical (T) Division and the Computational Physics and Methods (CCS-2) Group within the Computer, Computational, and Statistical Sciences (CCS) Division. Before joining the Laboratory in August 2020, he was a postdoc under the mentorship of Tom Manteuffel at the University of Colorado, Boulder. Ben's research interests are broad in numerical analysis, numerical linear algebra, and numerical PDEs, with a particular interest in applying principles from diverse fields of research to develop faster and more accurate numerical methods.

Ben earned a B.S. in mathematics from Dartmouth College and a Ph.D. in applied mathematics at the University of Colorado at Boulder. Ben is co-mentored David Moulton of T-5, and James Warsa of CCS-2.

Innovative Applications of Block Preconditioning and Fast Linear Solvers

Fast linear solvers (e.g., multigrid) and block preconditioning are well-studied and widely used techniques in the numerical simulation of partial differential equations (PDEs). After the spatial domain of a given problem has been discretized, such methods are fundamental to rapidly solving the linear(ized) set of equations that defines the solution at the next time step or in equilibrium. Here, we consider new perspectives on fast linear solvers and block preconditioning, developing new solutions to old yet unanswered problems in PDEs, and also applying the principles of linear and nonlinear preconditioning to new areas. In particular, we consider the development and application of efficient implicit-explicit and multirate time integration schemes for multiscale PDEs, and the development of fast training schemes for data science models.

Current and Past
Metropolis Postdoc Fellows

Name	Postdoc Org(s)	Current Org
Burke, Timothy	XCP-3	XCP-3
Charest, Marc	XCP-8	XCP-1
Cheng, Roseanne	CCS-2 XCP-2 T-1	T-1
Collins, David C	T-2 T-5 XTD-3	N/A
Dhakal, Tilak	XCP-2 T-3 XCP-6	FICO
Dolence, Joshua	CCS-2 XTD-IDA	CCS-2
Ellinger Carola	CCS-2 XCP-2 XTD-IDA	CCS-7
Haines, Brian	XCP-2 XCP-4	XCP-2
Jadrich, Ryan	T-1	T-1
Josey, Colin	XCP-3	XCP-3
Kinch, Brooks	CCS-2	N/A
Krueger, Brendan	CCS-2 XTD-IDA	XCP-2
Larkin, Kevin*	XCP-1 XCP-5	XCP-1 XCP-5
Lovegrove, Elizabeth	XCP-1 CCS-2	N/A

*Current Metropolis Fellow

Current and Past
Metropolis Postdoc Fellows
Continued

Name	Postdoc Org(s)	Current Org
	CCS-2	
Malone, Chris	XTD-IDA	XCP-1
Manzanares, Adam	HPC-5	N/A
	CCS-3	
Miller, Robyn	CCS-7	N/A
	XTD-NTA	
	T-2	
Nelson, Nick	XCP-4	N/A
Pavel, Robert	CCS-7	CCS-7
	T-3	
	T-1	
Petsev, Nikolai	C-PCS	N/A
Phillips, Johsua	T-6	N/A
Smith, Justin	T-1	T-1
	CCS-2	
Smullen, Rachel	XTD-IDA	XTD-IDA
	T-5	T-5
Southworth, Ben*	CCS-2	CCS-2
	XCP-6	
Taitano, William	T-5	T-5
Ticknor, Christopher	T-1	T-1
Till, Andrew	CCS-2	CCS-2
	T-3	
Willert, Jeff	XTD-IDA	N/A

*Current Metropolis Fellow

POSTDOC PROGRAM

LA-UR-22-XXXXX